2-(Methylsulfanyl)quinoxaline
21948-73-2 | DTXSID00325902

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.91e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.00e-01

Confidence level: 6.30e-01

Nearest Neighbors from the Training Set

Image not found

2,2',4,4',5-Pentabromodiphenyl ether
Measured: 1.80e-05
Predicted: 4.14e-08

Image not found

1,2,4,7,8-Pentachlorodibenzofuran
Measured: 4.00e-06
Predicted: 1.96e-09

Image not found

Pentylcyclohexane
Measured: 2.00e-06
Predicted: 6.06e-01

Image not found

Bibenzyl
Measured: 3.61e-04
Predicted: 7.42e-03

Image not found

Indole
Measured: 2.99e-02
Predicted: 1.60e-02